Critical behavior of the fully frustrated q-state Potts piled-up-domino model

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A q-state fully frustrated Potts model, the piled-up-domino model, is studied for different integer and noninteger values of q. Phase diagrams and some critical exponents are calculated using numerical transfer matrix methods. Foster, Gérard, and Puha [J. Phys. A **34**, 5193 (2001)] have shown that there is a reentrant paramagnetic phase when $q=3$. It is shown here that the direction of reentrance changes as q passes through $q=2$ and disappears for a certain value of $q=q^*$. The phase diagram of the model is radically different for $q<q^*$ and $q>q^*$. Tentative numerical results suggest $q^* \approx 4$.

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I. INTRODUCTION

The effects of frustration in spin models have been of considerable interest for a couple of decades, partly because of the rich critical behavior which arises and partly because frustration is considered an important feature of the behavior of spin glasses. Frustration arises when competing interactions prevent the system from simultaneously minimizing all its local interactions.[1] In general frustration gives rise to infinitely degenerate ground states.[2,3] The type of critical behavior seen is related, not to the symmetry group of the spins, but to the symmetry of the model as a whole, made larger by frustration and indicated by the infinite degeneracy of the ground state.

About twenty years ago, André *et al.*[4] introduced two periodically frustrated Ising models on a square lattice, the piled-up-domino model, and the zigzag model (the names refer to the patterns formed by the ferromagnetic and antiferromagnetic interactions). There are two obvious generalizations to these models; the first consists of replacing the Ising spins by spins of symmetry $O(n)$. This path was followed for the case of XY spins $[O(n=2)]$,[5] leading to a controversy over the critical behavior expected.[6–8] Foster, Gérard, and Puha[9] followed the alternative path of replacing the Ising spins with three-state Potts spins. Of particular interest was the Potts piled-up-domino model, which was found to have very different critical behavior when compared to the equivalent Ising model. Notably the three-state Potts model has a reentrant paramagnetic phase absent from the Ising model equivalent. The exact phase diagram is shown, as a function of $\alpha=J_2/J_1$, for the Ising piled-up-domino model in Fig. 1 while a schematic phase diagram for the three-state Potts piled-up-domino model, summarizing the results of Ref. 9, is shown in Fig. 2. In this article we extend the piled-up-domino model to general values of q.

Since the behavior changes when q is changed from 2 to 3 it is natural to ask how the phase diagram changes as q is varied continuously. If there are other changes of behavior, what are the values of q for which these changes occur? It is known, for example, that $q=4$ is special for the standard ferromagnetic Potts model ($J_1=J_2>0$), corresponding to the value of q for which the transition changes from critical to first order.[10,11] It is also known that $q=3$ is a special value for the mixed ferroantiferromagnetic Potts model, where the transition is thought to be of Kosterlitz-Thouless type,[12,13] and beyond which there is no transition.[14] In this paper we will investigate these points in detail using the numerical transfer matrix and finite-size-scaling methods, described in the next section.

It turns out that at least two special values of q may be identified. The first is $q=2$; for $q<2$ the paramagnetic phase enters under the ordered phase from the right while for $2<q<q^*$ the paramagnetic phase enters from the left (see Figs. 2 and 6). Beyond some value of $q=q^*$ the reentrance disappears, and the two transition lines are now replaced by a single first-order transition line. In the next section the model and the numerical methods used are presented. In Sec. III we present our results and the paper closes with concluding remarks in Sec. IV.

II. MODEL AND CALCULATION METHODS

The q-state Potts model is defined as a set of variables $\{\sigma_i\}$ associated with the sites $\{i\}$ of a lattice.[15] Each σ_i takes one of q distinct values. The Hamiltonian of the model is given by

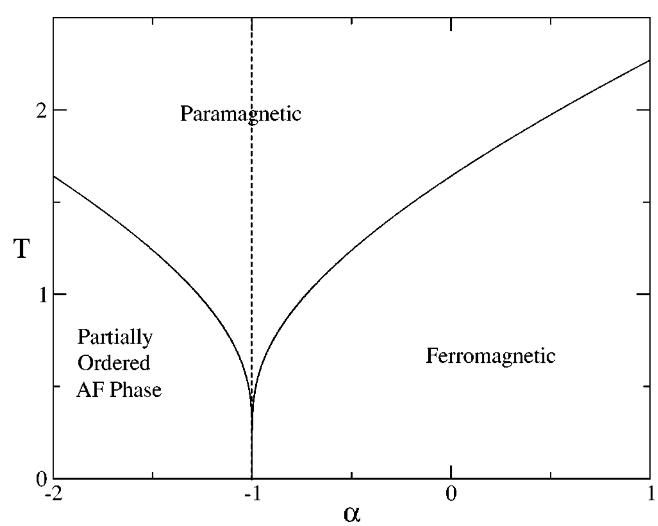

FIG. 1. The exact phase diagram as a function of $\alpha=J_2/J_1$ for the Ising piled-up-domino model as found by André *et al.*[4]

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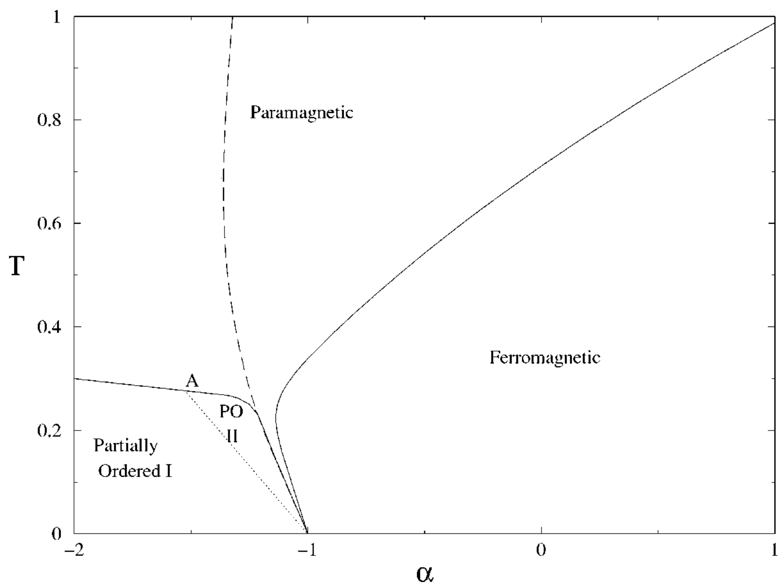

FIG. 2. Schematic phase diagram as a function of $\alpha = J_2/J_1$ for the $q=3$ Potts piled-up-domino model as proposed by Foster *et al.* (Ref. 9). We will argue here that the phase POII does not exist as a thermodynamic phase.

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{i,j}\delta_{\sigma_i,\sigma_j}, \tag{1}$$

where the sum runs over all pairs of sites and $J_{i,j}$ are the interaction strengths between a given pair of spins. For the piled-up-domino model, of interest in this article, the interaction strengths are given by

$$J_{i,j} = \begin{cases} 0 & \text{for non-nearest-neighbor spins,} \\ J_1 & \text{for nearest-neighbor (NN) spins along the solid lines,} \\ J_2 & \text{for NN spins along the dashed lines,} \end{cases} \tag{2}$$

as shown in Fig. 3. For convenience we define $\alpha = J_2/J_1$. J_1 will be taken as positive (ferromagnetic) throughout.

The model as given here is only defined for integer values of q. It is, however, possible to extend the model to noninteger values of q by expressing the partition function in terms of its graphical expansion. This mapping proceeds exactly as in the ferromagnetic case, well explained in Ref. 11, and gives the partition function in terms of the graphs of bond linked clusters as follows:

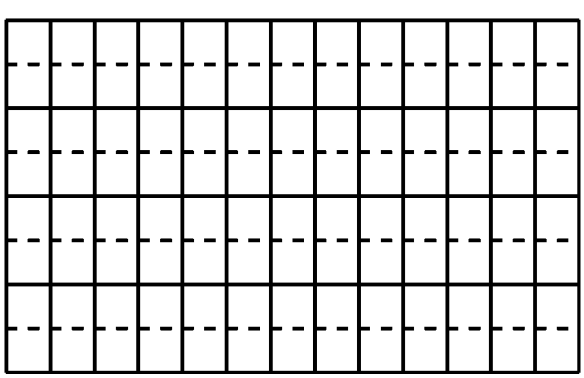

FIG. 3. Arrangement of the nearest-neighbor interactions defining the Potts piled-up-domino model: the interaction energy is J_1 along the solid lines and J_2 along the dashed lines.

$$\mathcal{Z} = \sum_{\text{clusters}} \left(\frac{u_1}{q}\right)^{N_1}\left(\frac{u_2}{q}\right)^{N_2} q^C, \tag{3}$$

where N_1 and N_2 are the numbers of occupied bonds corresponding to the interaction bonds J_1 and J_2, respectively, $u_1 = \exp(\beta J_1) - 1$ and $u_2 = \exp(\beta J_2) - 1$, where $\beta = 1/kT$, and C is the number of nonconnected clusters. In this formulation the value of q enters as a parameter with the same standing as the other model parameters such as u_1 and u_2, and so it is natural to extend the model to real values of q.

The main results presented in this paper were obtained using transfer matrix methods. The locality of the interactions in the model enables a rewriting of the partition function for a lattice of length N and width L as follows:

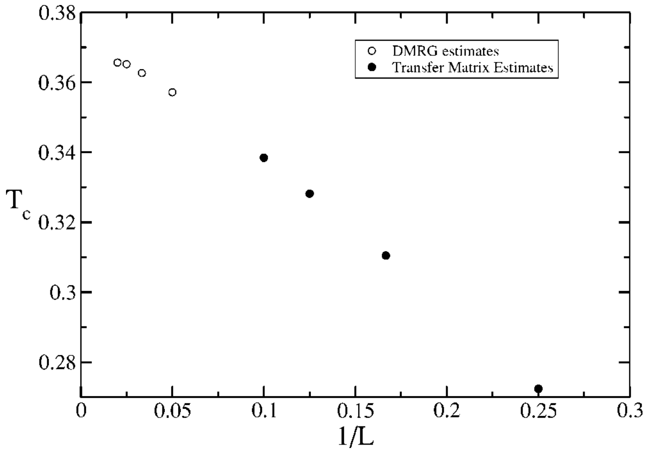

FIG. 4. Finite-size estimates for the critical temperature T_c calculated using DMRG and transfer matrices, taking $\alpha=-1$ and $q=3$ calculated using 8 with $L'=L+2$.

$$\mathcal{Z}_{L,N}=\sum_{\{\sigma_{x,y}\}}\prod_{x=1,N}\exp[-\beta\mathcal{E}(\{\sigma_{(x-1,y)},\sigma_{(x,y)}\})], \tag{4}$$

where $\mathcal{E}$ is the energy contribution due to the interactions between the spins in column $x-1$ and column x and half the energy contribution from the spins within columns $x-1$ and x. The factor one-half for the energy due to the spin-spin interactions within a column is chosen to avoid double counting when the product in Eq. (4) is performed. Equation (4) is most neatly expressed in matrix form

$$\mathcal{Z}_{L,N}=\mathrm{Tr}\mathcal{T}^N, \tag{5}$$

where the transfer matrix $\mathcal{T}=\exp(-\beta\mathcal{E})$, has been introduced and periodic boundary conditions are taken in the x direction. Equation (5) may be written in terms of the eigenvalues of $\mathcal{T}$. It is easy to show, by taking the limit $N\to\infty$, that the dimensionless free energy per spin f and the correlation length ξ for an infinitely long strip of width L are given by

$$f_L=\frac{1}{L}\ln\lambda_0, \tag{6}$$

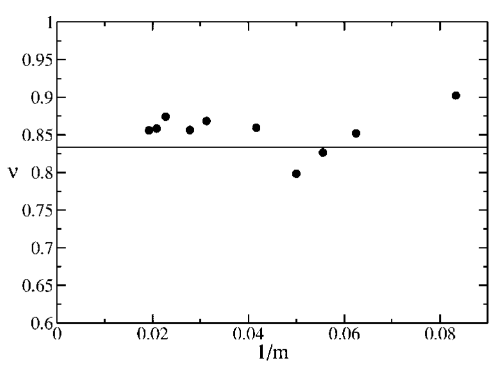

FIG. 5. Estimates for the critical exponent ν using DMRG with $\alpha=-1$, $q=3$ with $L=50$, $L'=52$. m is a measure of the number of states kept at each DMRG iteration (for full definition see text). The horizontal line shows the value of ν for the standard three-state ferromagnetic Potts model ($\nu=5/6$.).

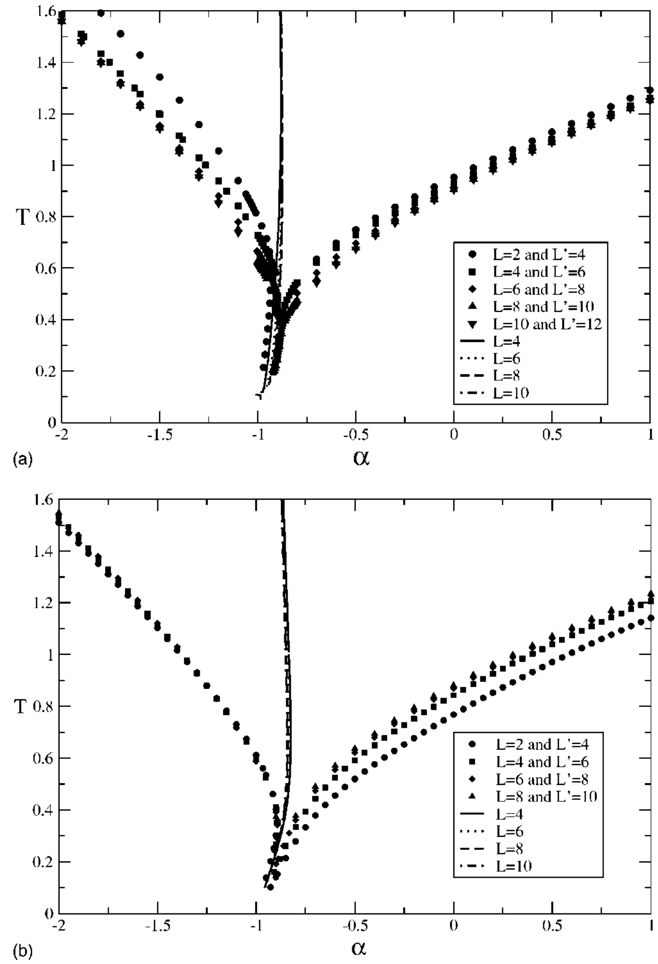

FIG. 6. The phase diagram for $q=1.5$ found using transfer matrices and the phenomenological renormalization group with (a) periodic and (b) free boundary conditions. The points correspond to finite-size estimates for T_c, while the lines correspond to the estimates for the disorder line ($\alpha=J_2/J_1$).

$$\xi_L=\frac{1}{\ln\left(\frac{\lambda_0}{|\lambda_1|}\right)}, \tag{7}$$

where λ_0 and λ_1 are, respectively, the eigenvalues with the largest and second largest absolute values of $\mathcal{T}$.

The phase diagram may be found using the phenomenological renormalization group, where finite size critical temperature estimates are associated with solutions of the equation[16]

$$\frac{\xi_L}{L}=\frac{\xi_{L'}}{L'}. \tag{8}$$

This approach relies on the expected scale invariance at criticality in the thermodynamic limit. In this limit, the correlation length is expected to have a power law behavior, described by

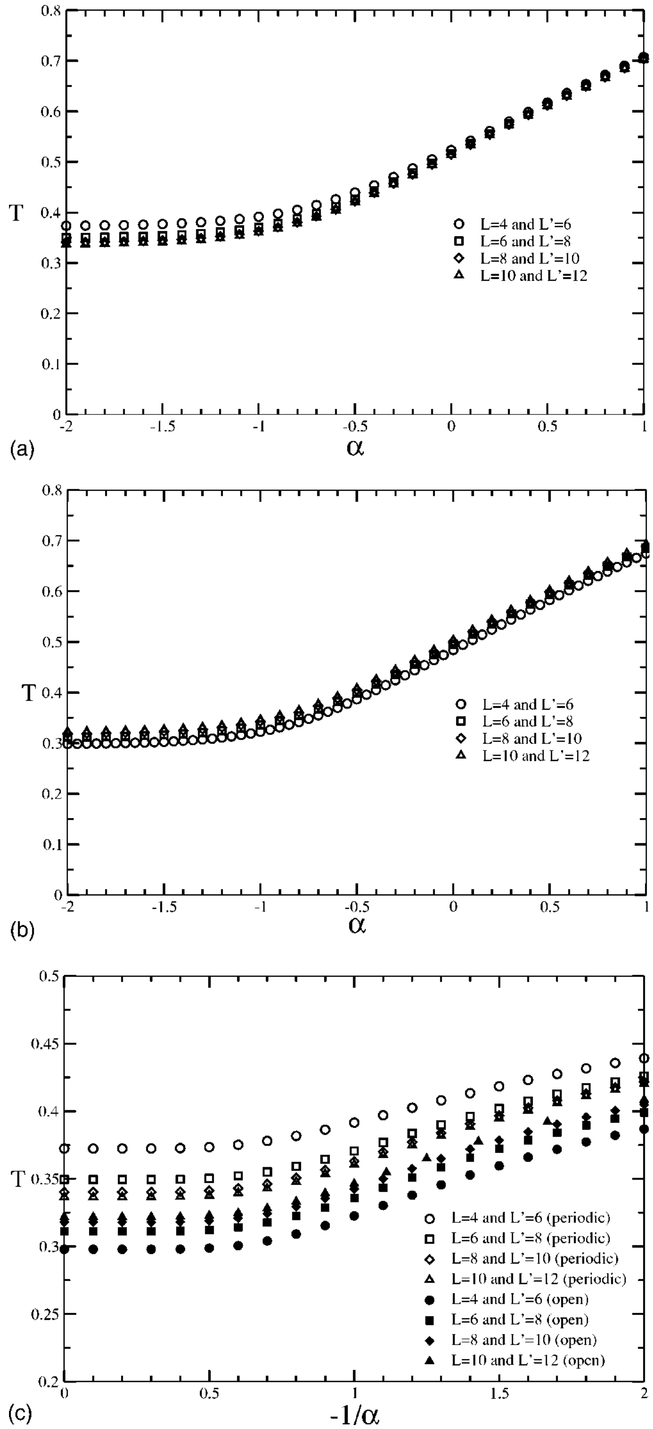

FIG. 7. Estimates of the thermal exponent $y_T=1/\nu$ for $q=10$ and $q=64$ for $\alpha=0$ and $\alpha=1$ as a function of $1/L$ with $L'=L+2$.

$$\xi=|T-T_c|^{-\nu}, \tag{9}$$

where ν is the correlation length critical exponent and T_c is the critical temperature. Using standard finite-size scaling arguments, finite-size estimates of ν are given by

$$\frac{1}{\nu_{L,L'}}=\frac{\ln\left(\frac{\partial \xi_L}{\partial T}/\frac{\partial \xi_{L'}}{\partial T}\right)}{\ln(L/L')}+1. \tag{10}$$

TABLE I. Finite-size estimates of T_c and ν for (a) periodic boundary conditions and (b) free boundary conditions with $q=1.5$ for three values of $\alpha=J_2/J_1$, calculated using transfer matrices and finite-size scaling.

	T_c		
L/L'	$\alpha=-2$	$\alpha=-1$	$\alpha=1$
	(a)		
4/6	1.586114	0.728082	1.261419
6/8	1.563152	0.663427	1.253856
8/10	1.560069	0.627152	1.251955
10/12	1.559307	0.60741	1.251281
	(b)		
4/6	1.532177	0.599232	1.206717
6/8	1.542430	0.587361	1.227032
8/10	1.547948	0.581704	1.235888
10/12	1.551212	0.579152	1.240528
∞	1.559 ± 0.001	0.575 ± 0.005	1.250 ± 0.003[a]
	ν		
L/L'	$\alpha=-2$	$\alpha=-1$	$\alpha=1$
	(a)		
4/6	0.945744	0.525958	1.087435
6/8	0.981070	0.613453	1.108565
8/10	0.975370	0.688523	1.116414
10/12	0.970590	0.745299	1.120403
	(b)		
4/6	0.989166	0.881934	1.143539
6/8	0.983198	0.957554	1.147167
8/10	0.974492	1.003521	1.148211
10/12	0.969478	1.016751	1.141964
∞	0.957 ± 0.002	$\cdots$	1.126 ± 0.002[b]

[a]Exact critical temperature for $q=1.5$ is $T_c=1/\log(1+\sqrt{1.5})=1.250559\cdots$ (Ref. 11).
[b]Estimate found using only the results for periodic boundary conditions, exact result gives $\nu\approx1.128$ (Ref. 19).

III. RESULTS

As discussed in the Introduction, the Ising version of the piled-up-domino model was studied by André *et al.*,[4] who gave the exact phase diagram, shown in Fig. 1. The three-state Potts piled-up-domino model was investigated using transfer matrix methods by Foster, Gérard, and Puha.[9] The phase diagram proposed in Ref. 9 for the three-state Potts piled-up-domino model is shown schematically in Fig. 2. Later we will argue that the phase denoted POII in Fig. 2 is likely to be a numerical artifact.

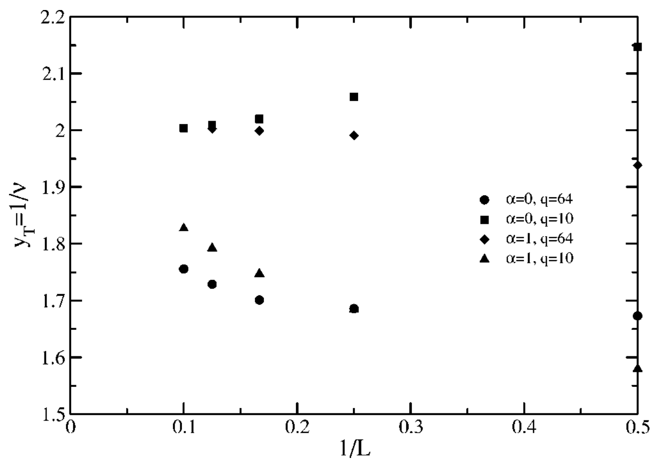

FIG. 8. The phase diagram for $q=10$ found using transfer matrices and the phenomenological renormalization group with (a) periodic, (b) free boundary conditions for $-2<\alpha<1$, and (c) the phase diagrams extended to $\alpha \to -\infty$ (open symbols represent periodic boundary conditions and closed symbols represent open boundary conditions). The points give the finite-size estimates for T_c $(\alpha=J_2/J_1)$.

The model is of particular interest when $\alpha=-1$. For this value of α the frustration effects are strongest, giving rise to a maximum in the ground-state entropy. The point $T=0$, $\alpha=-1$ remains an important point in the three-state Potts piled-up-domino model, but, as a result of the observed reentrance, there is another transition at nonzero temperature. In Ref. 9, the estimated value of T_c for $\alpha=-1$ is given as 0.37 ± 0.01. The values of ν reported were consistent with the transition being of the Potts ferromagnetic type, but the finite-size estimates were still far from their limiting values.

The three-state Potts model lends itself to the use of the density matrix renormalization group method (DMRG). For classical spin models, DMRG amounts to an iterative approximation method for calculating the dominant eigenvalues of the transfer matrix. DMRG thus allows the construction of approximate transfer matrices for much larger system sizes than are accessible to standard transfer matrix calculations. The method works by judicious pruning of phase space by repeated projection onto a prototype system composed of a strip of width four spins; the inner two spins are the original model spins while the outer spins are m-state spins introduced to represent, approximately, the rest of the original system. Clearly the value of m chosen determines the amount of information which may be kept from one iteration to the next, and hence the quality of the approximation. For a detailed description of the method, the reader is referred to Refs. 17 and 18.

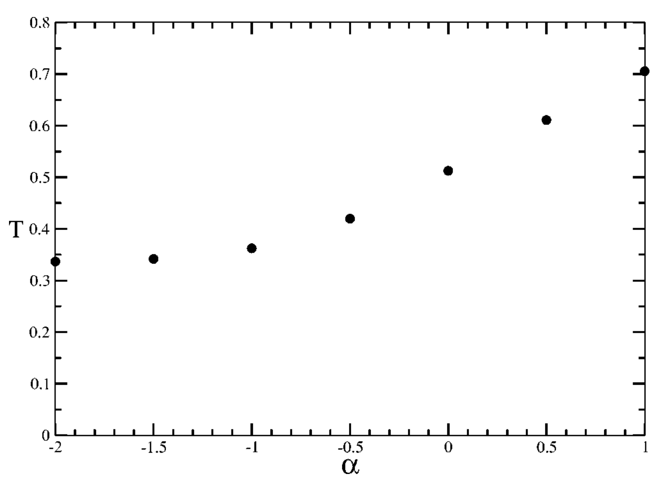

FIG. 9. Phase diagram for $q=10$ calculated using the Monte Carlo histogram method for a system of size 40×40 with periodic boundary conditions.

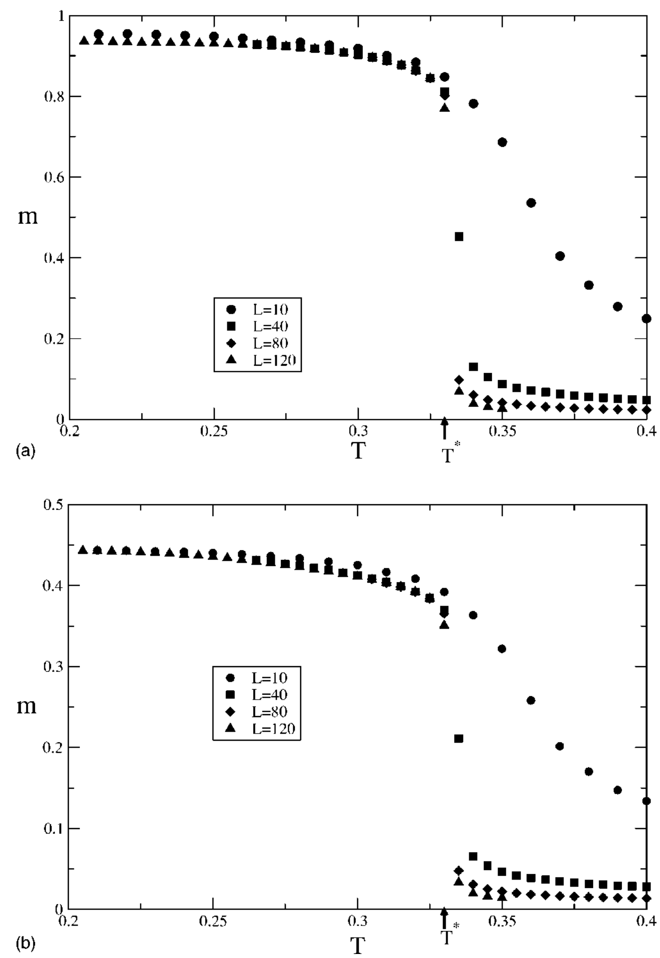

FIG. 10. The magnetization plotted as a function of temperature for $q=10$ and $\alpha=-2$ along (a) the lines of ferromagnetic interactions and (b) the lines of antiferromagnetic interactions. The magnetization seems to be developing a jump discontinuity, consistent with a first-order transition. The estimated transition temperature T^* estimated from transfer matrices is indicated.

We applied the DMRG method to the $q=3$ Potts piled-up-domino model with free boundary conditions for lattice widths up to $L=52$ for $\alpha=-1$ in order to obtain improved estimates of T_c. For a given lattice width, m was varied and extrapolated to ∞ to obtain finite-size estimates for T_c. These estimates are shown in Fig. 4. This gives a new estimate for $T_c=0.365\pm0.001$. The calculations were performed taking the J_2 interactions parallel to the transfer (x) direction. Commensurability problems arise as a result of the frustration, which results in certain values of m better representing the

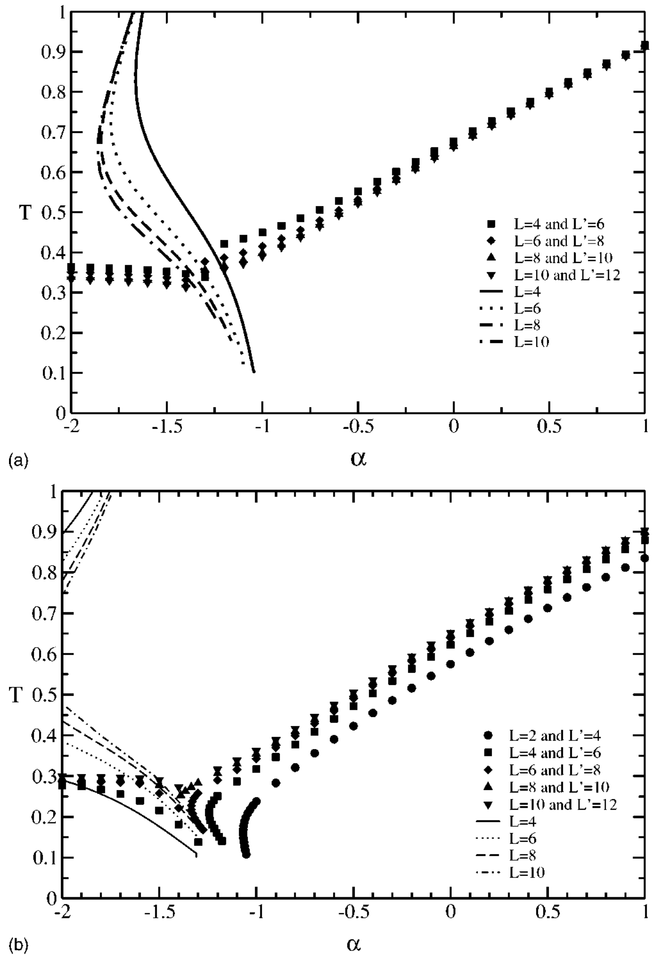

FIG. 11. The phase diagram for $q=4$ found using transfer matrices and the phenomenological renormalization group with (a) periodic and (b) free boundary conditions. The points correspond to finite-size estimates for T_c, while the lines correspond to the estimates for the disorder line ($\alpha=J_2/J_1$).

system than other, possibly larger, values of m. While these effects are not particularly strong for the calculation of T_c, they are more noticeable for the calculation of ν. While the estimates of ν decrease with L, strong fluctuations as a function of m prevent a quantitative extrapolation with lattice size. In Fig. 5 the results for $L=50$ and $L'=52$ (the largest sizes reached) are shown. All that can confidently be stated is that the results are compatible with the pure Potts result, $\nu=5/6$. As a result of these strong fluctuation effects, in what follows we shall limit ourselves to using standard transfer matrices, which, while limited by system size, have the advantage of being numerically exact for the given value of L.

It is natural to ask how the phase diagram changes as the value of q is changed from $q<2$ to $q>2$. In Fig. 6 we show the phase diagram for $q=1.5$. There is still a reentrant paramagnetic phase, and so a non-zero T_c for $\alpha=-1$. The transition is no longer in the ferromagnetic Potts universality class. For $\alpha=1$ we find a value of $\nu=1.126\pm0.002$ (Ref. 19) while for $\alpha=-2$ we find $\nu=0.957\pm0.002$. Finite size estimates for T_c and ν for $q=1.5$ are given in Table I. Also shown in Fig. 6 is the disorder line. The disorder line is defined as the line at which the correlation function changes from being monotonic to oscillatory, to reflect the underlying ferromagnetic or antiferromagnetic behavior.[20] It correponds necessarily to a minimum of the correlation length measured along some direction. The disorder line may not cut a critical line (where the correlation length is infinite). The form of the disorder line estimates are consistent with the proposed critical lines, terminating at the special point $T=0$, $\alpha=-1$.

For the ferromagnetic Potts model the nature of the phase transition is different for $q\leqslant4$ and $q>4$.[11] In the former case the transition is critical while in the latter case the transition is first order. This first-order nature is in general difficult to see numerically for values of q close to 4, but more clearly seen for $q\approx10$. Since the nature of the phase transition for the ferromagnetic line to the right of $\alpha=-1$ changes, it is relevant to ask if there may be an equivalent change in the phase transition to the left of $\alpha=-1$. In order to answer this question we investigate the phase diagram for $q=10$.

Despite the first-order nature of the transition for $q>4$, estimates for the transition lines may still be found using Eq. (8), at least for the pure Potts case ($\alpha=1$), since it is expected that the transition is described by a discontinuity fixed point, with an effective exponent $\nu=1/d=1/2$.[21] Blöte and Nightingale showed that the discontinuity fixed-point exponent is more difficult to extract than the standard critical exponent.[22] For the infinite strip geometry convergence to $\nu=1/d$ is only found if the temperature is fixed to the known critical temperature and finite size scaling of $d\xi/dT$ is examined using Eq. (10).[22] Convergence improves for higher values of q are used. For our model, the critical temperature is known for two values of α, namely, $\alpha=1$ (the pure Potts model) and $\alpha=0$.[9] Estimates for the thermal exponent $y_T=1/\nu$ are shown in Fig. 7 for $\alpha=0$ and $\alpha=1$ for $q=10$ and $q=64$. The convergence to the expected discontinuity fixed point value, $y_T=d$ is very good for $q=64$ in both cases, whilst for $q=10$ the convergence is slower, but nevertheless reasonably convincing. Since there is no sign of a change of behavior as a function of α, it is reasonable to suppose that the entire transition line is described by the same discontinuity fixed point, and that it is reasonable to use a finite-size scaling approach to find it. The phase diagram for $q=10$ is shown in Fig. 8.

There are two features of the phase diagram for $q=10$ which are of particular interest. The first is that the reentrance has disappeared. This picture is confirmed by the form of the disorder lines, which for $q=10$ do not cross the transition line, but rather are split into two branches, one above and one below the transition line. The disorder lines are not shown in Fig. 8 since the upper branch is outside the scale of the diagram. The low temperature phase is now ferromagnetic for all values of α. The two transition lines present for $q=3$ are now replaced, for $q=10$, by only one transition line, which is first-order, since the transition for $\alpha=1$ is first order.[11]

To verify the picture of only one first order phase transition, results of Monte Carlo simulations are shown in Figs. 9 and 10. In Fig. 9 we show the phase diagram calculated using the histogram method for a lattice size of 40×40 with periodic boundary conditions, which confirms the general shape of the phase diagram found using transfer matrices. In

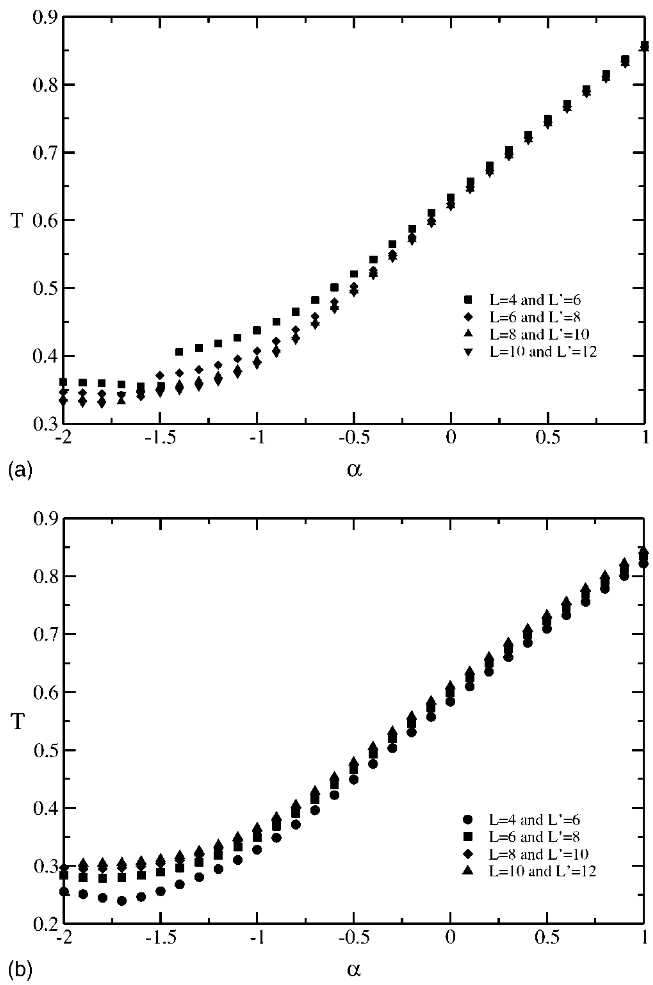

FIG. 12. The phase diagram for $q=1.5$ found using transfer matrices and the phenomenological renormalization group with (a) periodic and (b) free boundary conditions. $\alpha=J_2/J_1$.

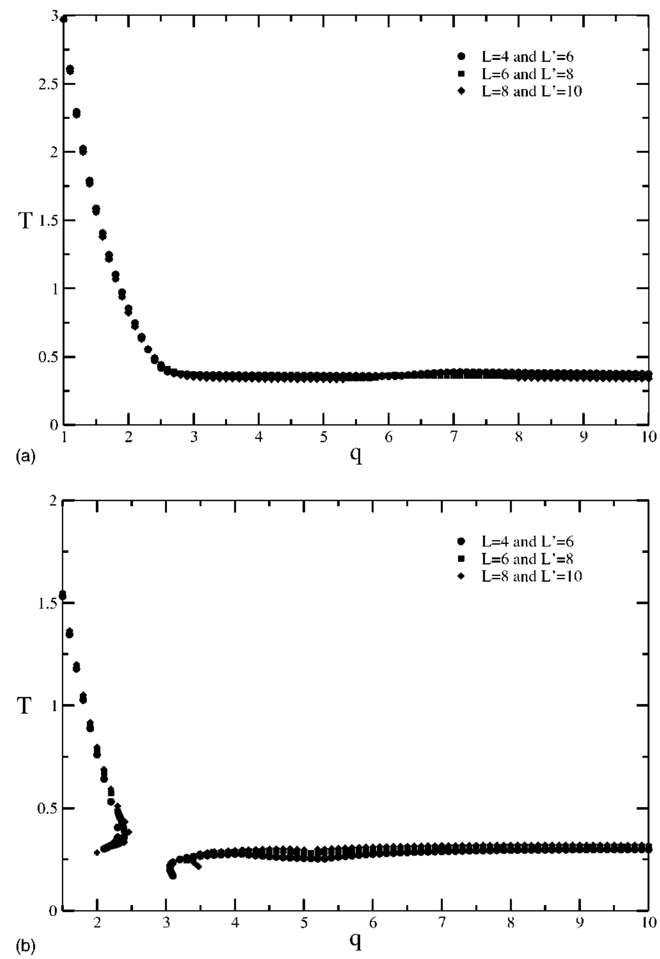

FIG. 13. Estimates of the transition temperature T_c using tranfer matrices, as a function of q with (a) periodic and (b) free boundary conditions for $\alpha=-2$.

order to confirm the suspected first order nature of the transition line far from the usual ferromagnetic model ($\alpha=1$), we show in Fig. 10 plots of the Potts magnetization, defined through

$$m = \frac{1}{q-1}(q\langle n_{\max}\rangle - 1), \tag{11}$$

where $n_{\max}=N_{\max}/N$. $N_{\max}$ is the number of spins in the most represented spin state in a group of N spins. The group of spins taken is usually all the spins on the lattice, whereas for our purposes it is more convenient to calculate magnetizations separately along the lines of ferromagnetic and antiferromagnetic interactions. The magnetization is plotted in Fig. 10 for sites for ferromagnetic (J_1 interacting) and antiferromagnetic (J_2 interacting) rows for $\alpha=-2$. The ferromagnetic rows have the standard ferromagnetic behavior seen for $\alpha=1$. The antiferromagnetic rows, however, do not saturate to 1 as the temperature goes to zero. This is an indication that some of the spins remain partially disordered. Closer investigation reveals that the low temperature phase is one in which alternate spins along the even (J_2) lines order, and the others do not. Due to translational invariance, Fig. 10(b) shows an average of these two types of spin. The order parameter seems to be developing a jump discontinuity at the transition temperature, again consistent with the proposed first-order behavior. The temperature at which the magnetization jumps is consistent with the transition temperature

TABLE II. Finite-size estimates for T_c for (a) periodic boundary conditions and (b) free boundary conditions calculated using transfer matrices with $q=10$ and $\alpha=-2$

L/L'	(a) T_c	(b) T_c
4/6	0.373448	0.298713
6/8	0.350440	0.312203
8/10	0.341196	0.318899
10/12	0.337639	0.322777
∞	0.330 ± 0.005	

$T^*=0.330\pm0.005$ as estimated using transfer matrices (see Table II).

The results shown clearly indicate that there must exist a value of $q=q^*$ where the frustration-induced phase transition for $\alpha<-1$ disappears, to be replaced by the standard (first-order) phase transition for all values of α. Figures 11 and 12 show the phase diagrams for $q=4$ and $q=5$, respectively. While the results are less clear than for $q=10$ and $q=3$, there are indications that for $q=5$ there is no reentrant phase. The periodic boundary conditions show a remnant of the reentrant phase, but which seems to vanish as the system size is increased. This is confirmed by the disorder lines (not shown) which split into two distinct lines as for the $q=10$ case. For $q=4$, however, while the periodic boundary conditions show a vanishing jump where the reentrant phase is expected, there seems to be a limiting "kink." The free boundary conditions confirm this picture, where the reentrant phase does not seem to vanish, but rather becomes narrower with increasing size. The finite-size evolution of the disorder lines show clearly that in the limit of infinite system size, there will be a limiting line which would have to cross the transition line if there were only one, again indicating the presence of two transition lines with possibly a vanishingly narrow reentrant paramagnetic phase.

In Fig. 13 we show estimates for the transition temperature as a function of q for periodic and free boundary conditions for $\alpha=-2$. It may be seen that there is no solution to the phenomenological renormalisation group [Eq. (8)] for a range of values of q, at least for the lattice sizes considered here. The size and position of this zone without solution evolves with lattice size, and since the solution lines may not end in the middle of nowhere, there are nonphysical extensions of the solution lines, giving rise to apparent double transitions for some values of q. For $\alpha=-2$ it is seen that there is no solution for $q=3$, but for appropriate values of α there exist two solutions, one physical and the other almost certainly not. This is clearly the explanation for the observed extra phase (POII) shown in Fig. 2, reported in Ref. 9.

Figure 14 shows the critical temperature estimates in the limit $\alpha\to-\infty$, which corresponds to setting $u_2=-1$ in Eq. (3). The critical temperature for $q\leqslant2$ is infinite in this limit. For $q>2$ the transition temperature (critical or not depending on the value of q) is finite, explaining the very flat transition line for $\alpha<-1$ for these values of q.

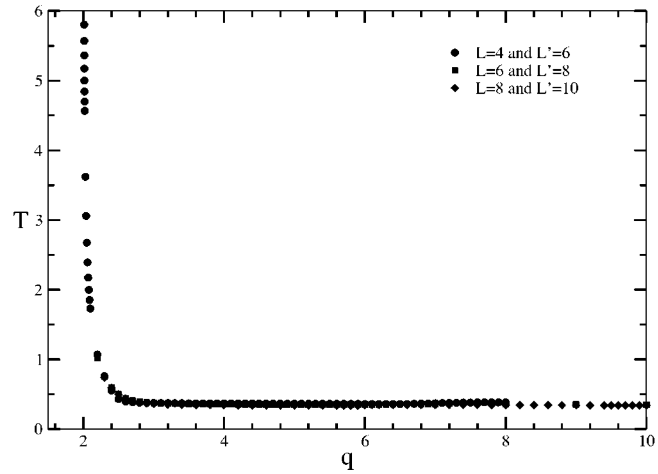

FIG. 14. Estimates of the transition temperature T_c using transfer matrices, as a function of q with periodic boundary conditions and $\alpha=-\infty$.

IV. CONCLUSION

In this article we present a variety of results showing that the critical behavior of the frustrated Potts piled-up-domino model is rich and far from trivial. We confirm the existence of a transition at finite temperature for $q=3$ and $\alpha=-1$ and improve the accuracy of the determination of the critical temperature using DMRG. However, the main results of this article relate to the rich variety of behaviours observed as q is varied.

(1) For $q<2$, $T_c\to\infty$ as $\alpha\to-\infty$, and there is a reentrant paramagnetic phase which enters under the partially ordered phase.

(2) For $q=2$, $T_c\to\infty$ as $\alpha\to-\infty$, but there is no reentrant paramagnetic phase and $T_c=0$ for $\alpha=-1$.

(3) For $q^*>q>2$, T_c remains finite as $\alpha\to-\infty$, and the reentrant phase enters under the ferromagnetic phase.

(4) There exists some value $q^*>3$ such that for $q\geqslant q^*$ the reentrant phase disappears, to be replaced by a single line of first-order transitions for all values of α.

There are many questions left unanswered, for example the nature of the criticality around $q=3$ and the value of q^*. We have shown that there is some indication that q^* is around 4.

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